

STN Columbus

***** Welcome to STN International *****

NEWS 1 Web Page for STN Seminar Schedule - N. America
 NEWS 2 OCT 02 CA/Caplus enhanced with pre-1907 records from Chemisches
 Zentralblatt
 NEWS 3 OCT 19 BEILSTEIN updated with new compounds
 NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
 NEWS 5 NOV 19 WPIX enhanced with XML display format
 NEWS 6 NOV 30 ICSD reloaded with enhancements
 NEWS 7 DEC 04 LINPADOODB now available on STN
 NEWS 8 DEC 14 BEILSTEIN pricing structure to change
 NEWS 9 DEC 17 USPATOLD added to additional database clusters
 NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
 NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
 NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
 MEDLINE segment
 NEWS 13 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
 NEWS 14 DEC 17 CA/Caplus enhanced with new custom IPC display formats
 NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
 from USPATOLD
 NEWS 16 JAN 02 STN pricing information for 2008 now available
 NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
 prophetic substances
 NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
 custom IPC display formats
 NEWS 19 JAN 28 MARPAT searching enhanced
 NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
 of publication
 NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
 NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
 NEWS 23 FEB 08 STN Express, Version 8.3, now available
 NEWS 24 FEB 20 PCI now available as a replacement to DPCI
 NEWS 25 FEB 25 IFIREF reloaded with enhancements
 NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
 NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
 U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
 AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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 NEWS IPC8 For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 22:16:47 ON 26 MAR 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 22:16:58 ON 26 MAR 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1
 DICTIONARY FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> e rapamycin/cn
E1      1      RAPAMMUNE/CN
E2      1      RAPAMUNE/CN
E3      1 --> RAPAMYCIN/CN
E4      1      RAPAMYCIN 29-ENOL/CN
E5      1      RAPAMYCIN 31-O-METHYLTRANSFERASE/CN
E6      1      RAPAMYCIN 42-(BENZYL SUCCINATE)/CN
E7      1      RAPAMYCIN 42-(METHYL SUCCINATE)/CN
E8      1      RAPAMYCIN 42-HEMIADIPATE/CN
E9      1      RAPAMYCIN 42-HEMISUCCINATE/CN
E10     1      RAPAMYCIN ASSOCIATED PROTEIN (CARASSIUS AURATUS FRAGMENT)/CN
E11     1      RAPAMYCIN ASSOCIATED PROTEIN FRAP2 (HUMAN CLONE 99P18 GENE F
E12     1      RAP2 C-TERMINAL FRAGMENT)/CN
E12     1      RAPAMYCIN DIACETATE/CN
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=> s e3
```

```
L1      1 RAPAMYCIN/CN
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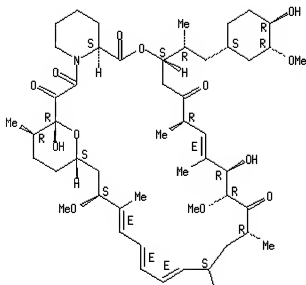
```
=> d
```

```
L1      ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN      53123-88-9 REGISTRY
ED      Entered STN: 16 Nov 1984
CN      Rapamycin (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN      23,27-Epoxy-3H-pyrido[2,1-c][1,4]oxaazacyclohentrriacontine, rapamycin
      deriv.
OTHER NAMES:
CN      (-)-Rapamycin
CN      (3S,6R,7E,9R,10R,12R,14S,15E,17E,19E,21S,23S,26R,27R,34aS)-
      1,5,11,28,29(4H,6H,31H)-pentone, 9,10,12,13,14,21,22,23,24,25,26,27,32,33,34,34a-Hexadecahydro-9,27-
      dihydroxy-3-[1R]-2-[1S,3R,4R]-4-hydroxy-3-methoxycyclohexyl]-1-
      methylethyl]-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-23,27-epoxy-3H-
      pyrido[2,1-c][1,4]oxaazacyclohentrriacontine-1,5,11,28,29(4H,6H,31H)-
      pentone
CN      23,27-Epoxy-3H-pyrido[2,1-c][1,4]oxaazacyclohentrriacontine-
      1,5,11,28,29(4H,6H,31H)-pentone, 9,10,12,13,14,21,22,23,24,25,26,27,32,33,
      34,34a-hexadecahydro-9,27-dihydroxy-3-[2-(4-hydroxy-3-methoxycyclohexyl)-1-
      methylethyl]-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-,
      [3S-[3R*[S*(1R*,3S*,4S*)],6S*,7E,9S*,10S*,12S*,14R*,15E,17E,19E,21R*,23R*,
      26S*,27S*,34aR*)]]-
CN      Antibiotic AY 22989
CN      AY 22989
CN      NSC 226080
CN      RAPA
CN      Rapammune
CN      Rapammune
CN      RPM
CN      SIIA 9268A
CN      Sirolimus
```

CN Wy 090217
 CN [3S-[3R*[S*(1R*,3S*,4S*)],6S*,7E,9S*,10S*,12S*,14R*,15E,17E,19E,21R*,23R*,
 26S*,27S*,34aR*)]-9,10,12,13,14,21,22,23,24,25,26,27,32,33,34,34a-
 Hexadecahydro-9,27-dihydroxy-3-[2-(4-hydroxy-3-methoxycyclohexyl)-1-
 methylethyl]-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-23,27-epoxy-3H-
 pyrido[2,1-c][1,4]oxaazacyclohentriacontine-1,5,11,28,29(4H,6H,31H)-
 pentone
 FS STEREOSEARCH
 MF C51 H79 N O13
 CI COM
 LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS,
 BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN,
 CSCHEM, DDFU, DRUGU, EMBASE, HSDB*, IFCDB, IFIPAT, IFIUD, IMSDRUGNEWS,
 IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS,
 NAPRALERT, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE,
 TOXCENTER, USAN, USPAT2, USPATFULL, VETU
 (*File contains numerically searchable property data)
 Other Sources: WHO

Absolute stereochemistry.
 Double bond geometry as shown.

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PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5162 REFERENCES IN FILE CA (1907 TO DATE)
 325 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 5194 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file merck
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
7.61	7.82

FILE 'MRCK' ENTERED AT 22:17:20 ON 26 MAR 2008
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L2 1 L1

=> d all

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MERCK Number (MNO): 8202

CAS Registry No. (RN): 53123-88-9

MERCK Index Name (MIN): Rapamycin

Synonym(s) (CN): Sirolimus; RAPA; RPM

Drug Code(s) (CN): AY-22989; NSC-226080

Trade Name(s) (CN): Rapamune (Wyeth)

Molecular Form. (MF): C51 H79 N O13

Wgt Composition (COMP): C 67.01%, H 8.71%, N 1.53%, O 22.75%.

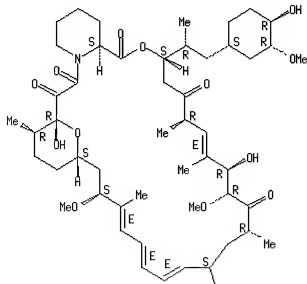
Molecular Weight (MW): 914.17

References (RE): Triene macrolide antibiotic isolated from *Streptomyces hygroscopicus*. Name derived from the native word for Easter Island, Rapa Nui. Isoln: S. N. Sehgal et al., DE 2347682; eidem, US 3929992 (1974, 1975 both to Ayerst McKenna Harrison); purification and characterization: C. Vezina et al., J. Antibiot. 28, 721 (1975); S. N. Sehgal et al., ibid. 727. Inhibition of immune response: R. R. Martel et al., Can. J. Physiol. Pharmacol. 55, 48 (1977); of graft rejection in mice: C. P. Eng et al., Transplant. Proc. 23, 868 (1991). Total synthesis: K. C. Nicolaou et al., J. Am. Chem. Soc. 115, 4419 (1993); D. Romo et al., ibid. 7906. Series of articles on therapeutic monitoring and pharmacokinetics: Clin. Ther. 22, Suppl. 2, B1-B132 (2000); on pharmacology and clinical experience in transplantation: Transplant. Proc. 35, Suppl. 1, S1-S233 (2003). Clinical trial in prevention of coronary restenosis: D. R. Holmes, Jr. et al., Circulation 109, 634 (2004).

Absolute stereochemistry.

Double bond geometry as shown.

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PAGE 2-A



Melting Point (MP):

Value
MP
deg C

183 - 185

Optical Rotatory Power (ORP):

Value	Temp.	Line	Spectral	Note
ORP	ORP.T	ORP.SL		
deg	deg C			
-58.2	25	D		(methanol)

Toxicity (TOX):

LD50 in mice (mg/kg): 600 i.p.; >2,500 orally (Vezina).

UV Spectrum (UVS):

Peak Pos.	Maximum	Note
UVS.PP		
nm		
267		(95% ethanol) (E1%1cm 417, 541, 416)
277		
288		

Other Properties (OCPP):

Colorless crystalline solid from ether, mp 183-185°. uv max (95% ethanol): 267, 277, 288 nm (E1%1cm 417, 541, 416). [α]D₂₅ -58.2° (methanol). Sol in ether, chloroform, acetone, methanol and DMF; very sparingly sol in hexane and petr ether. Substantially insol in water. LD50 in mice (mg/kg): 600 i.p. ; > 2,500 orally (Vezina)

Application (APP):

Tool for immunochemistry.

Therapeutic Codes (THER):

Immunosuppressant; antirestenotic.

Referenced Patent (RPN):

DE2347682; US3929992

=> log y

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

3.47

11.29

STN INTERNATIONAL LOGOFF AT 22:18:55 ON 26 MAR 2008